Alternate grids for diffusion weighted imaging and associated reconstruction algorithms

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Introduction

Many problems in physics, mathematics and engineering involve integration and interpolation on the sphere in $\mathbb{R}^3$. Of particular importance are discretizations of rotationally invariant subspaces of $L^2(\mathbb{S}^2)$ that integrate all spherical harmonics up to a fixed order and degree. Typically, the sphere is discretized using equally spaced nodes in azimuthal angle and Gauss-Legendre nodes in polar angle, leading to an unreasonably dense concentration of nodes near the poles. In a variety of applications such concentration of nodes may lead to problems when using these grids. Alternatively, Sobolev [2] suggested the use of grids that are invariant under finite rotation groups. In such constructions there is no clustering of nodes and, moreover, the number of nodes necessary to integrate a particular subspace is close to optimal.

We develop a systematic numerical approach for constructing nearly optimal quadratures invariant under the icosahedral group to integrate rotationally invariant subspaces of $L^2(\mathbb{S}^2)$ up to a fixed order and degree. Using these grids and a reproducing kernel, we show how to replace the standard basis of spherical harmonics by a representation formed using a single function centered at the quadrature nodes. The reproducing kernel is mostly concentrated near the corresponding grid point. In this representation, the coefficients, up to a factor, are the values on the grid of the function being represented. We may interpret this construction as an analogue of Lagrange interpolation on the sphere.

We view our approach as the first step in constructing a local and multiresolution representation of functions on the sphere that respects rotationally invariant subspaces.

Preliminaries

Here we establish notation and state some well known results about spherical harmonics, reproducing kernels and state two theorems by Sobolev.

We denote the unit sphere in $\mathbb{R}^3$ as $\mathbb{S}^2$. An orthonormal basis for $L^2(\mathbb{S}^2)$ is given by the spherical harmonics,

$$Y_n^m(\theta,\phi) = \frac{1}{\sqrt{2\pi}}\overline{P}_n^m(\cos\theta)e^{im\phi},\ 0 \le |m| \le n, \quad n = 0,1,\ldots, \tag{1}$$

where the polar angle $\theta \in [0,\pi]$, the azimuthal angle $\phi \in [0,2\pi)$ and $\overline{P}_n^m$ are the normalized associated Legendre functions. We define a subspace of spherical harmonics with fixed degree n as

$$\mathcal{H}_n = \mathrm{span}\left\{Y_n^m(\theta,\phi),\ |m| \le n\right\}. \tag{2}$$

The dimension of $\mathcal{H}_n$ is $2n+1$. The subspace of maximum degree N is then the direct sum

$$\mathcal{P}_N = \bigoplus_{n=0}^{N}\mathcal{H}_n = \mathrm{span}\left\{Y_n^m(\theta,\phi),\ |m| \le n,\ 0 \le n \le N\right\} \tag{3}$$

and has dimension $(N+1)^2$. The reproducing kernel for $\mathcal{P}_N$,

$$K(\boldsymbol{\omega}\cdot\boldsymbol{\omega}') = \sum_{n=0}^{N}\frac{2n+1}{4\pi}P_n(\boldsymbol{\omega}\cdot\boldsymbol{\omega}'), \tag{4}$$

satisfies

$$f(\boldsymbol{\omega}) = \int_{\mathbb{S}^2}K(\boldsymbol{\omega}\cdot\boldsymbol{\omega}')f(\boldsymbol{\omega}')\,d\Omega',\quad f \in \mathcal{P}_N. \tag{5}$$

The identity in (5) may be verified by using the addition theorem for spherical harmonics. We rely on (5) to develop a representation of functions in $\mathcal{P}_N$ which is an analogue of Lagrange interpolation on the sphere, known as hyper-interpolation.

Sobolev's paper [2] contains two key results that we now summarize, specialized to the icosahedral rotation group:

Theorem 1. *Let Q be a quadrature rule invariant under the group G. Then Q is exact for all functions $f \in \mathcal{P}_N$ if and only if Q is exact for functions f invariant under G.*

This theorem reduces the size of the system of nonlinear equations which must be solved to determine a quadrature invariant under the group G. The next result gives a formula to calculate the number of invariant functions under the group G in a subspace of spherical harmonics $\mathcal{H}_n$ of a given degree n. Let $q_1 = 5$ be the number of edges meeting at a vertex of an icosahedron, $q_2 = 3$ be the number of sides of its (triangular) face and $q_3 = 2$ denote the order of rotation about mid-points of opposing edges.

Theorem 2. *For a given degree n, the number of functions invariant under the icosahedral rotation group in a subspace of spherical harmonics $\mathcal{H}_n$ is given by*

$$S(n) = \left\lfloor\frac{n}{q_1}\right\rfloor + \left\lfloor\frac{n}{q_2}\right\rfloor + \left\lfloor\frac{n}{q_3}\right\rfloor - n + 1,$$

where $\lfloor\ \rfloor$ denotes the integer part.

Quadratures for the sphere

The main difficulty in constructing quadratures comes from the need to solve a large system of nonlinear equations. Without using special structure of these equations, general root finding or optimization methods typically fail. The essence of our approach is to develop and use such structure within a root finding method.

To start, there are four different types of orbits of the icosahedral rotation group. In general, a point on the sphere under the action of the group generates a total of 60 points. However, if a point is a vertex of the icosahedron, then it generates a total of only 12 distinct points. Also, if a point is the projection of the center of an icosahedral face onto the sphere, it generates 20 distinct points in total. Finally, if a point is the projection onto the sphere of the mid-point of an edge, it generates a total of 30 distinct points. When describing these different types of orbits it is sufficient to consider a single point, a generator of its orbit. The orbit of a point with spherical coordinates (θ,ϕ) is the set $\left\{\left(g_i^{-1}\theta, g_i^{-1}\phi\right)\ |\ g_i \in G\right\}$ and, depending on the type of orbit, has cardinality 12, 20, 30 or 60.

With these types of orbits in mind, we consider four types of quadratures. The first type assumes that all generators, except for a vertex of the icosahedron, give rise to orbits of size 60, i.e.,

$$Q_v(f) = w_v\sum_{i=1}^{12}f(\theta_i^v,\phi_i^v) + \sum_{j=1}^{N_g}w_j\sum_{i=1}^{60}f(\theta_i^{(j)},\phi_i^{(j)}), \tag{6}$$

where $\left\{\theta_i^v,\phi_i^v\right\}_{i=1}^{12}$ are coordinates of the vertices of an icosahedron inscribed in the unit sphere, w_v their associated weight, N_g is the number of generators with coordinates $\left\{\theta^{(j)},\phi^{(j)}\right\}_{j=1}^{N_g}$ and weights $\left\{w_j\right\}_{j=1}^{N_g}$. For each $g_i \in G$, we denote $\left(\theta_i^{(j)},\phi_i^{(j)}\right) = \left(g_i^{-1}\theta^{(j)}, g_i^{-1}\phi^{(j)}\right)$.

The second type of quadrature has the form

$$Q_{vf}(f) = w_v\sum_{i=1}^{12}f(\theta_i^v,\phi_i^v) + w_f\sum_{i=1}^{20}f\left(\theta_i^f,\phi_i^f\right) + \sum_{j=1}^{N_g}w_j\sum_{i=1}^{60}f\left(\theta_i^{(j)},\phi_i^{(j)}\right), \tag{7}$$

where $\left\{\theta_i^f,\phi_i^f\right\}_{i=1}^{20}$ are coordinates of the face centers of the icosahedron projected onto the sphere and w_f is the associated weight.

The other quadratures are constructed in a similar manner. Using Theorem 2, we determine the number of invariant functions in the subspace $\mathcal{H}_n$. Theorem 1 allows us to limit the number of equations to not exceed the number of invariant functions. We solve the resulting system of equations using Newton's method.

Figure 1 shows a type 1 quadrature for $\mathcal{P}_{145}$ with 7121 nodes.

A useful way of measuring the efficiency of a quadrature is the ratio of the dimension of the subspace to be integrated to the (maximum) number of degrees of freedom in the quadrature rule (two coordinates and a weight for each node):

$$\eta = \frac{(N+1)^2}{3M}, \tag{8}$$

where M is the number of nodes. If $\eta = 1$, we call the quadrature optimal. In Figure 2 we display the potential efficiency of quadrature Q_v as a function of the degree N of subspace $\mathcal{P}_N$ using Theorem 2 to count invariants and superimpose the actual efficiencies of computed quadratures. The behavior of efficiency of other quadratures is similar. For comparison, efficiency of the standard quadrature $\eta = 2/3$ is also shown. Solid dots indicate the efficiency of computed quadratures using our approach.

Local representations

Using the new quadratures, we construct an alternative representation for functions on invariant subspaces of $L^2(\mathbb{S}^2)$ by discretizing Eq. (5)

$$f(\boldsymbol{\omega}) = \sum_{j=1}^{M}K(\boldsymbol{\omega}\cdot\boldsymbol{\omega}_j)w_jf(\boldsymbol{\omega}_j). \tag{9}$$

If $f \in \mathcal{P}_N$, then (9) provides an exact reconstruction of the function f from its values $f(\boldsymbol{\omega}_1), f(\boldsymbol{\omega}_2),\ldots, f(\boldsymbol{\omega}_M)$. The functions $\left\{K(\boldsymbol{\omega}\cdot\boldsymbol{\omega}_j)w_j\right\}_{j=1}^{M}$ play a role similar to that of Lagrange interpolating polynomials and, therefore, we may think of (9) as an analogue of Lagrange interpolation on the sphere.

Further localization of K may be achieved by optimization techniques.

Conclusions

We introduced a numerical method for constructing quadratures invariant under the icosahedral group which integrate rotationally invariant subspaces of $L^2(\mathbb{S}^2)$. Using these quadratures, an exact representation of functions on rotationally invariant subspaces of $L^2(\mathbb{S}^2)$, similar to Lagrange interpolation, was developed. The results of this paper are the first step to develop practical computational methods for applications that deal with the sphere. See [1] for more details.

References

[1] C. Ahrens and G. Beylkin. Rotationally invariant quadratures for the sphere. *Proceedings of the Royal Society A*, 465:3103–3125, 2009.

[2] S. L. Sobolev. Cubature formulas on the sphere invariant under finite groups of rotations. *Doklady Akademii Nauk SSSR*, 146:310–313, 1962.